Nuclear Criticality Safety Program
Technical Program Review
26-27 March 2014

LA-UR-14-21786

MCNP Progress
&
Performance Improvements

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Monte Carlo Codes, XCP-3

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Advanced Simulation & Computing™

NNSA Nuclear Criticality Safety Program

US DOE/NNSA Nuclear Criticality Safety Program –

What have we done for you lately ?

- **MCNP6.1 Release, with ENDF/B-VII.1**
- **Verification / Validation**
- **User Support & Training**
- **Performance Improvements**
- **Work in Progress**

MCNP6.1 Status (1)

Monte Carlo Codes
XCP-3, LANL

- **MCNP release by RSICC, July 2013**

MCNP6.1	– production version
MCNP5-1.60, MCNPX-2.70	– old versions, no changes
Nuclear Data Libraries	– including ENDF/B-VII.1 data
MCNP Reference Collection	– 600+ technical reports

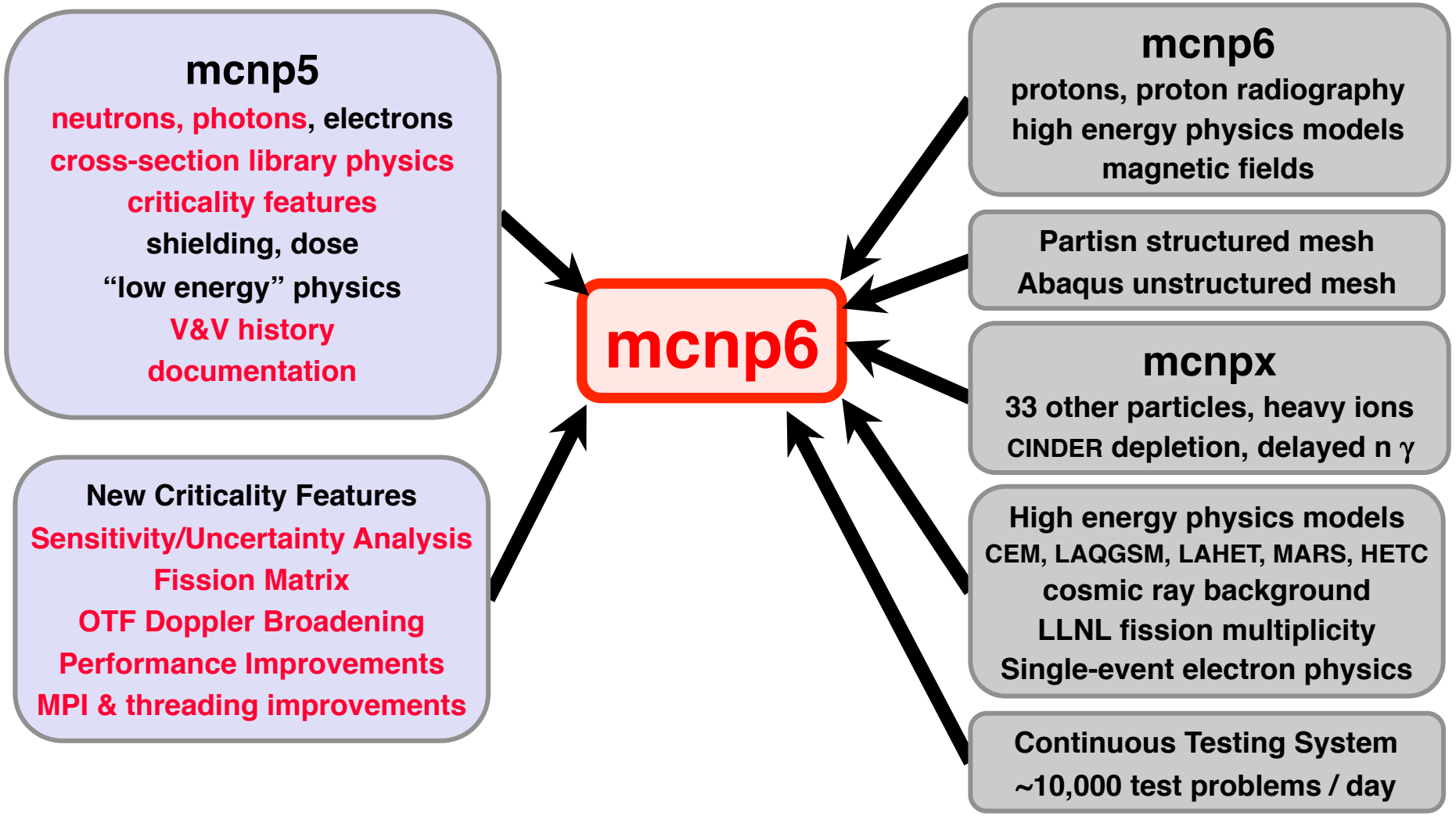
12,000+ copies of MCNP distributed 2001-2012
2,000+ copies of MCNP6 distributed 2013

- **MCNP6.1.1 – beta release, planned for June 2014**
  - Primarily for DHS users, no effect on crit-safety
  - Next production release targeted for 2015
- **MCNP5 & MCNPX are frozen – all new development & fixes are in MCNP6**
- **Criticality safety community needs to transition to MCNP6**

Support from DOE-NNSA-ASC, DOE-NNSA-NCSP, DOE, DoD, DTRA, DHS/DNDO, NASA, & others

MCNP6.1 Status (2)

Monte Carlo Codes
XCP-3, LANL



mcnp5 – 100 K lines of code

mcnp6 – 500 K lines of code

Verification & Validation (1)

We do a lot of verification/validation work - all the time, especially for MCNP6:

MCNP Verification-Validation, 100+ reports on MCNP Website

Verification of MCNP6.1 for Criticality Safety Applications, LA-UR-14-xxxxx, in progress (2014).

Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications, LA-UR-13-22196 (**2013**).

Verification of MCNP5-1.60 and MCNP6-Beta-2 for Criticality Safety Applications, LA-UR-12-210 (**2012**).

MCNP5-1.60 Release & Verification, Trans Am Nuc Soc 104, June 2011, LA-UR-11-00230 (**2011**).

ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks & Reactor Experiments, Nuclear Data Sheets, Vol 112, No. 12, 2997-3036 [LA-UR-11-11271] (**2011**).

An Expanded Criticality Validation Suite for MCNP, ICNC-2011, LA-UR-11-04170 (**2011**).

Verification of MCNP5-1.60, LA-UR-10-05611 (**2010**).

Nuclear Data

Listing of Available ACE Data Tables, LA-UR-13-21822 (**2013**)

Continuous Energy Neutron Cross Section Data ...ENDF/B-VII.1, LA-UR-13-20137 (**2013**).

LANL Data Testing Support for ENDF/B-VII.1, LA-UR-12-20002 (**2012**).

ENDF/B-VII.1 Nuclear Data....., Nuclear Data Sheets, Vol 112, No. 12, 2887-2996 (**2011**).

ENDF/B-VII.0: ... Nuclear Data ..., Nuclear Data Sheets, Vol. 107, Number 12 (**2006**)

New ACE-Formatted Neutron and Proton Libraries Based on ENDF/B-VII.0, LA-UR-08-1999 (**2008**).

Release of New MCNP S(α,β) Library ... ENDF/B-VII.0, LA-UR-08-3628 (**2008**).

Verification & Validation (2)

Monte Carlo Codes
XCP-3, LANL

Table 1. MCNP6.1 and MCNP6.1.1-Beta Results for Analytic Keff Benchmarks

Case	Name	Analytic keff	MCNP_Results keff	std
prob11	Ua-1-0-IN	2.25000	2.25000	0.00000
prob14	Ua-1-0-SP	1.00000	1.00006	0.00010
prob18	Uc-H2O(2)-1-0-SP	1.00000	1.00005	0.00011
prob23	UD2O-1-0-CY	1.00000	1.00000	0.00006
prob32	PUa-1-1-SL	1.00000	0.99995	0.00011
prob41	UD2Ob-1-1-SP	1.00000	1.00003	0.00007
prob44	PU-2-0-IN	2.68377	2.68377	0.00003
prob54	URRa-2-0-SL	1.00000	1.00007	0.00013
prob63	URRd-H2Ob(1)-2-0-ISLC	1.00000	0.99993	0.00006
prob75	URR-6-0-IN	1.60000	1.59999	0.00001

Results are identical for MCNP6.1 and MCNP6.1.1-Beta.

Wall-clock time, using 8 threads on Mac Pro:

MCNP6.1 151 min

MCNP6.1.1-beta 87 min

Verification & Validation (3)

Monte Carlo Codes
XCP-3, LANL

mcnp5-1.60 + ENDF/B-VII.0		mcnp5+Int-10	mcnp5_Int-11	mcnp5_Int-12	mcnp6_Int-12
		deltak std	keff std	deltak std	deltak std
U233 Benchmarks	JEZ233	0.0000 (8)	0.9989 (5)	0.0000 (8)	0.0000 (8)
	FLAT23	0.0000 (9)	0.9990 (7)	0.0000 (9)	0.0000 (9)
	UMF5C2	0.0000 (8)	0.9931 (5)	0.0000 (8)	0.0000 (8)
	FLSTF1	0.0000 (15)	0.9830 (11)	0.0000 (15)	0.0000 (15)
	SB25	0.0000 (14)	1.0053 (10)	0.0000 (14)	0.0000 (14)
	ORNL11	0.0000 (5)	1.0018 (4)	0.0000 (5)	0.0000 (5)
HEU Benchmarks	GODIVA	0.0000 (8)	0.9995 (5)	0.0000 (8)	0.0000 (8)
	TT2C11	0.0010 (10)	1.0008 (7)	0.0000 (9)	0.0000 (9)
	FLAT25	0.0000 (9)	1.0034 (7)	0.0000 (9)	0.0000 (9)
	GODIVR	0.0000 (9)	0.9990 (7)	0.0000 (9)	0.0000 (9)
	UH3C6	0.0000 (11)	0.9950 (8)	0.0000 (11)	0.0000 (11)
	ZEUS2	0.0002 (9)	0.9972 (7)	0.0000 (9)	0.0000 (9)
	SB5RN3	0.0000 (18)	0.9985 (13)	0.0000 (18)	0.0000 (18)
	ORNL10	0.0000 (5)	0.9993 (4)	0.0000 (5)	0.0000 (5)
IEU Benchmarks	IMF03	0.0000 (8)	1.0029 (5)	0.0000 (8)	0.0000 (8)
	BIGTEN	0.0000 (7)	0.9945 (5)	0.0000 (7)	0.0000 (7)
	IMF04	0.0000 (8)	1.0067 (5)	0.0000 (8)	0.0000 (8)
	ZEBR8H	-0.0001 (7)	1.0196 (5)	0.0000 (7)	0.0000 (7)
	ICT2C3	0.0000 (9)	1.0037 (7)	0.0000 (9)	0.0000 (9)
	STACY36	0.0000 (8)	0.9994 (5)	0.0000 (8)	0.0000 (8)
LEU Benchmarks	BAWXI2	0.0000 (9)	1.0013 (7)	0.0000 (9)	0.0000 (9)
	LST2C2	0.0000 (8)	0.9940 (5)	0.0000 (8)	0.0000 (8)
Pu Benchmarks	JEZPU	0.0000 (8)	1.0002 (5)	0.0000 (8)	0.0000 (8)
	JEZ240	0.0000 (8)	1.0002 (5)	0.0000 (8)	0.0000 (8)
	PUBTNS	0.0000 (8)	0.9996 (5)	0.0000 (8)	0.0000 (8)
	FLATPU	0.0000 (9)	1.0005 (7)	0.0000 (9)	0.0000 (9)
	THOR	0.0000 (9)	0.9980 (7)	0.0000 (9)	0.0000 (9)
	PUSH2O	0.0000 (9)	1.0012 (7)	0.0000 (9)	0.0000 (9)
	HISHPG	0.0004 (7)	1.0118 (5)	0.0000 (8)	0.0000 (8)
	PNL2	0.0000 (12)	1.0046 (9)	0.0000 (12)	0.0000 (12)
	PNL33	0.0000 (9)	1.0065 (7)	0.0000 (9)	0.0000 (9)
Wall-clock:		34.7 min	34.0 min	30.5 min	38.5 min
Rel. Speed:		0.98	1.00	1.11	0.88

Verification & Validation (4)

VERIFICATION_KEFF Suite – 10 analytical problems with exact K_{eff} results

- MCNP6.1, Intel-12 F90 — All results match

VALIDATION_CRITICALITY Suite – 31 ICSBEP Cases, ENDF/B-VII.0

- MCNP5 Intel-10 vs Intel-12: — 4 diffs, within statistics
- MCNP5 & MCNP6, Intel-12: — All results match

VALIDATION_CRIT_EXPANDED Suite – 119 ICSBEP Cases, ENDF/B-VII.0

Shortened Problems

- MCNP5 Intel-10 vs Intel-12: — 1 diff, within statistics
- MCNP5 & MCNP6, Intel-12: — All results match

Standard Problems

- MCNP5 & MCNP6, Intel-12: — 4 diffs, within statistics

CRIT_LANL_SBCS Suite – 194 ICSBEP Cases, ENDF/B-VI

MCNP5 vs MCNP6, Intel-10.1: — 187 match, 4 diffs < 1σ, 3 diffs < 2σ

MCNP5 (2013, Intel-12) vs
MCNP5 (2003, Intel-9) — 142 match, 42 diffs < 1σ, 10 diffs < 2σ

Verification & Validation (5)

- **Very thorough testing of MCNP6.1 on many computer platforms:**

  Brown, Kiedrowski, Bull, "Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications", LA-UR-13-22196 (2013).

  Conclusion: MCNP6.1 is solid & reliable for crit-safety calculations

- **MCNP6.1 impact on criticality calculation results ➜ none**
  - **All MCNP5 KCODE criticality features preserved, + new features**
  - **Matches results with MCNP5 for criticality suites**

- **Current MCNP6.1.1 beta exactly matches MCNP6.1 for crit-safety**

- **MCNP6.1 is 20-30% slower than MCNP5**
  - **Performance improvements address this, later in this talk**
  - **MCNP6.1.1 speed is comparable to or faster than MCNP5**

User Support & Training (1)

Monte Carlo Codes
XCP-3, LANL

- **12,000+ copies of MCNP distributed 2001-2012**
  2,000+ copies of MCNP6 distributed 2013

  MCNP Forum - User-group, beginners & experts, >1000 members

- **Classes**
  - **Theory & Practice of Criticality Calculations with MCNP**
    - FY13: 3 classes (including special class for LANL NCS group certification)
    - FY14: 2 classes (both with some LANL NCS staff)
  - **Introduction to MCNP** – 5 classes FY13, 5 classes FY14
  - **Advanced Variance Reduction** – 1 class each FY
  - **Intro + Variance Reduction** – Kirtland AFB 2014

- **Conferences & Journals**
  - **M&C 2013, NCSD 2013, SNA+MC 2013, PHYSOR 2014**
  - **ANS Washington, Reno, Anaheim**

- **Other: website, reference collection, summer students**

Performance Improvements (1)

Monte Carlo Codes
XCP-3, LANL

- **MCNP6.1**
  - Preserves all criticality features
  - ENDF/B-VII.1 data libraries
  - RSICC release - July 2013
- **MCNP6 Status**
  - Many new capabilities
  - Last few years – focus on features, merger, testing, release
  - Needs upgrade of core software
- **Path forward – MCNP 2020**
  - Concerted effort to modernize the codebase, upgrade foundations
  - Goals: modular, flexible, faster
  - Necessary for MCNP to survive into the 2020's

MCNP 2020

- **Improve performance**
  - 30-50% slowdown for MCNP6.1
  - Goal: 2X speedup within 2 years
- **Upgrade core MCNP6 software**
  - Restructure, clean up coding
  - Reorganize data structures
  - Evolution, not revolution
  - Reduce future costs for new development & maintenance
  - Goal: sustainable code
- **Prepare for future**
  - New computers – massive parallel but less memory per core
  - Improve MPI & thread parallelism
  - Goal: flexible, adaptable code

Performance Improvements (2)

- **Create a set of timing tests** ✔
  - Stress different portions of MCNP coding
  - Helps determine effect of specific code optimizations
- **Initial performance improvements** ✔
  - Eliminate strided f90 vector ops
  - Inline binary search, for neutron xsec routines
  - IF-guards, to avoid calling accessor functions
  - Inline code some other sections of coding
  - Eliminate unnecessary clearing of certain scratch arrays
  - Hash-based xsec energy lookups (algorithm change)
  - no work yet on tracking & geometry, or photon/electron routines
  - no work planned for any high energy physics
- **Intel compiler options** ✔
  - Higher Fortran optimization levels do not provide improvements
  - Using –O2 instead of –O1 provides only ~ 0-5% speedup, but some test problems segfault

Performance Improvements (3)

Tests run on Mac Pro, 3.0 GHz Xeon, 2 quad-cores, with 8 threads. ENDF/B-VII.1, discrete S(a,b)

CRITICALITY PROBLEMS

ks1.txt	3D PWR, OECD perf. bench., Kord Smith, 60 isotopes, no tallies
ks2.txt	ks1.txt, 10 isotopes, no tallies
ks3.txt	ks1.txt, 10 isotopes, fmesh tallies
ks4.txt	ks1.txt, 60 isotopes, fmesh tallies
baw1.txt	BAWXI2 ICSBEP problem, 31 isotopes, no tallies
baw2.txt	BAWXI2 ICSBEP problem, 31 isotopes, fmesh tallies
fvf.txt	fuel storage vault, from OECD convergence bencharks, 9 isotopes
g1.txt	Godiva problem, 3 isotopes
g2.txt	Godiva problem, 423 isotopes
pin.txt	AECL pin cell, with FPs, 147 isotopes

FIXED-SOURCE PROBLEMS

void1.txt	ks1.txt, with VOID card & no tallies
void2.txt	baw1.txt, with VOID card & no tallies
void3.txt	fvf.txt, with VOID card & no tallies
det1.txt	3D porosity tool, Reg. problem 12, neutrons, weight windows, F4 tallies
med1.txta	medical physics, modified 3D Zubal head, photons
pht1.txt	PHTVR cylindrical test problem, photons

Performance Improvements (4)

- **Speedups from recent performance improvements**

6/5 mcnp6.1 vs mcnp5

NEW/5 mcnp6.1.1 vs mcnp5

NEW/6 mcnp6.1.1 vs mcnp6.1

5: mcnp5-1.60

6: mcnp6.1, released

NEW: mcnp6.1,
+ no strides
+ inlining
+ if guards
+ thrd-priv. common
+ etc.
+ hash-based xs lookup

	----- Speedups -----		
Problem	6/5	NEW/5	NEW/6
Criticality			
ks1	0.88	1.54	1.76
ks2	0.40	0.85	2.13
ks3	0.63	0.85	1.35
ks4	0.72	0.98	1.36
baw1	0.44	0.97	2.19
baw2	0.58	0.93	1.59
fvf	0.38	0.77	2.04
g1	0.93	1.05	1.14
g2	0.82	1.80	2.20
pin	0.79	1.36	1.73
Other			
void1	0.24	0.72	3.03
void2	0.14	0.59	4.11
void3	0.26	0.71	2.72
det1	0.45	0.75	1.67
med1	0.57	0.65	1.15
pht1	0.58	0.71	1.22

- **Timing results for the standard VALIDATION_CRITICALITY test suite with ENDF-B/VII data**
  - Mac Pro (3 GHz, 8 cores), Intel 12.0 f90, run with 8 threads
  - Measured wall-clock times, including data I/O:

mcnp5	release	34.7 min
mcnp6.1	release	43.9 min
mcnp6	NEW	27.9 min

➜ 1.57 X speedup over mcnp6.1

➜ 1.24 X speedup over mcnp5

Speedups – NEW vs mcnp6.1

measured by Jeff Bull for mcnp performance test problems

Test	MCNP6 1.0 Release (min)	MCNP6 NEW (min)	Ratio
BAWXI2	63.58	14.55	4.37
mode p e in air	12.88	12.73	1.01
GODIVA	22.50	21.40	1.05
100M lattice cells in void	58.48	11.32	5.17
mode n p e in air	9.70	9.27	1.05
mode p in air	7.29	6.06	1.20
Pulse height tally	27.41	22.79	1.20
Radiography	33.30	31.06	1.07
Mode n in air with 750,000 tally bins	19.25	16.26	1.18
Well log (problem 12 from Regression suite)	57.89	30.27	1.91

Work in Progress (1)

MCNP 2020

- **Improve performance**
  - Focus on geometry tracking
- **Upgrade core MCNP6 software**
  - Restructure, clean up coding
  - Reorganize data structures
  - Evolution, not revolution
  - Reduce future costs for new development & maintenance
  - Goal: sustainable code
- **Prepare for future**
  - New computers – massive parallel but less memory per core
  - Improve MPI & thread parallelism
  - Goal: flexible, adaptable code

Parallel MPI & Threading

- **For criticality calculations**
  - Reduce the amount of data exchanged at MPI rendezvous
  - Tally server nodes
- **MPI improvements**
  - Eliminate synchronization
  - Asynchronous MPI messages
  - Improve Fortran/C interface
- **OpenMP threading improvements**
  - Replace private thread-safe storage for certain large arrays by OpenMP critical sections
  - Use OpenMP atomic operations with shared tally arrays

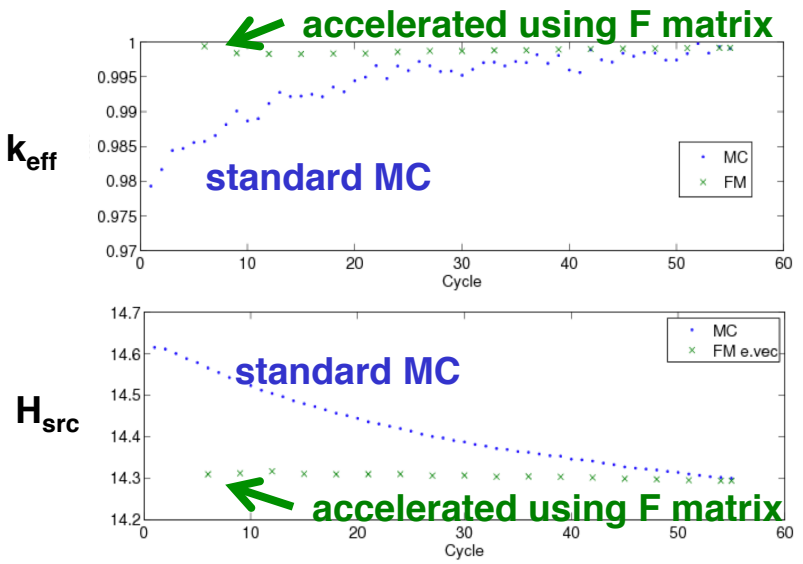
Work in Progress (2)

Physics & Temperature Dependence

- Implement modified free-gas scatter, to accurately model resonance upscattering for epithermal neutrons
- Full temperature dependence of S(a,b) thermal scattering
- Investigate coupling MCNP into multiphysics calculations

Fission Matrix

- Automatically determine source convergence, without user input
- Apply to subcritical multiplication problems
- Accelerate source convergence

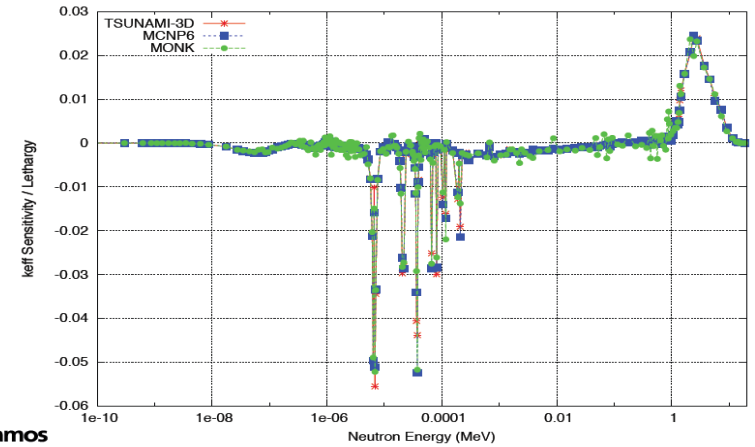


Work in Progress (3)

Continuous-energy Sensitivity/Uncertainty Analysis

- Uses adjoint-weighted perturbations
- Computes sensitivity coefficients for cross sections, fission, & scattering laws
- Can directly compare to TSUNAMI multigroup s/u results
- See Kiedrowski presentation

MOX Lattice: U-238 Total



Support for LANL PF-4 Nuclear Criticality Safety

- High priority
- See Kiedrowski presentation

Summary

- MCNP6.1 & ENDF/B-VII.1 released
- Impact on Criticality Calculations ➜ none
  - All KCODE criticality features same as for MCNP5
  - Matches results with MCNP5 for criticality suites
- Monte Carlo team will support MCNP6, no new features or releases of MCNP5 or MCNPX
- MCNP6 speed improved by 1.2 – 4 X for crit-safety
- More performance improvements in progress
- Criticality-safety community needs to plan for MCNP5 ➜ MCNP6 transition over the next few years